PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Mitigation of Knock and LSPI for High-Power Density Engines

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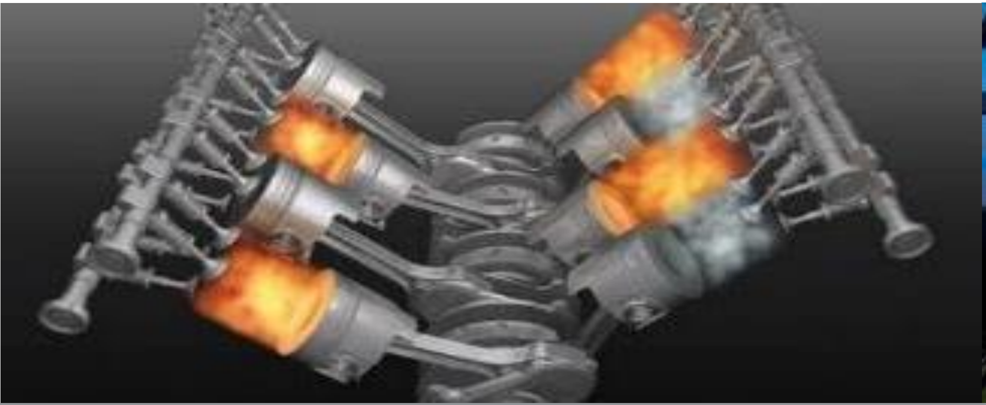
Oak Ridge National Laboratory

FY20 DOE Vehicle Technologies Office Annual Merit Review

June 2, 2020

Project # ACE147



This research was conducted as part of the Partnership to Advance Combustion Engines (PACE) sponsored by the U.S. Department of Energy (DOE) Vehicle Technologies Office (VTO). A special thanks to DOE VTO program managers Mike Weismiller and Gurpreet Singh.

Overview

Timeline

- **PACE started in Q3, FY19**
- **PACE will end in FY23 (~25% complete)**
- **Focus and objectives of individual tasks will be continuously adjusted**
- **Overall PACE work plan discussed in ACE138**

Budget

Presentations covers two FY20 PACE projects*

Task	FY19	FY20
F.01.02: Effectiveness of EGR to Mitigate Knock Throughout PT Domain (ORNL, Szybist)	$125k	$220k
F.01.03: Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI (ORNL, Splitter)	$100k	$220k

***FY20 outputs from these tasks feed into FY21 analysis tasks**

****Complete PACE budget in reviewer-only slides**

Barriers

USCAR Priority 1: Dilute SI Combustion

- **Knock Mitigation** → *Developing a better understanding of the effectiveness of EGR to mitigate knock*
- **Low speed preignition** → *Developing a better understanding of underlying mechanisms causing LSPI, as well as mitigation strategies*

PACE Major Outcome 1: Models to accurately predict knock
PACE Major Outcome 3: Phenomenological model of LSPI

Partners

- **PACE is a DOE-funded consortium of 6 National Laboratories working towards a common goal (ACE138)**
  - Goals and work plan developed considering input from stakeholders including DOE, ACEC Tech Team, CFD code developers, and more
- **Specific partners on this work include:**
  - LLNL on surrogate development and kinetics
  - Related LSPI funds-in project with CRC

Relevance

PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

PACE Purposes in ACE138

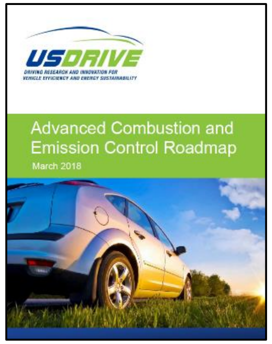
Overall Relevance of PACE:

PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions

Presentation Specific Relevance: PACE Major Outcomes 1 and 3

Major Outcome 1: Models for combustion system design accurately predict knock response to design changes → *Generating data for model validation*

Major Outcome 3: Develop new multi-step phenomenological mechanism for LSPI that captures wall-wetting, lubricant, and geometry effects → *Experiments to expand knowledge and understanding of LSPI*



Presentation Specific Relevance: USDRIVE ACEC Priority 1 for Dilute SI Combustion

Knock Mitigation → *Developing a better understanding of the effectiveness of EGR to mitigate knock*

Lowspeed Preignition → *Developing a better understanding of underlying mechanisms causing LSPI, as well as mitigation strategies*

*https://www.energy.gov/sites/prod/files/2018/03/f49/ACEC_TT_Roadmap_2018.pdf

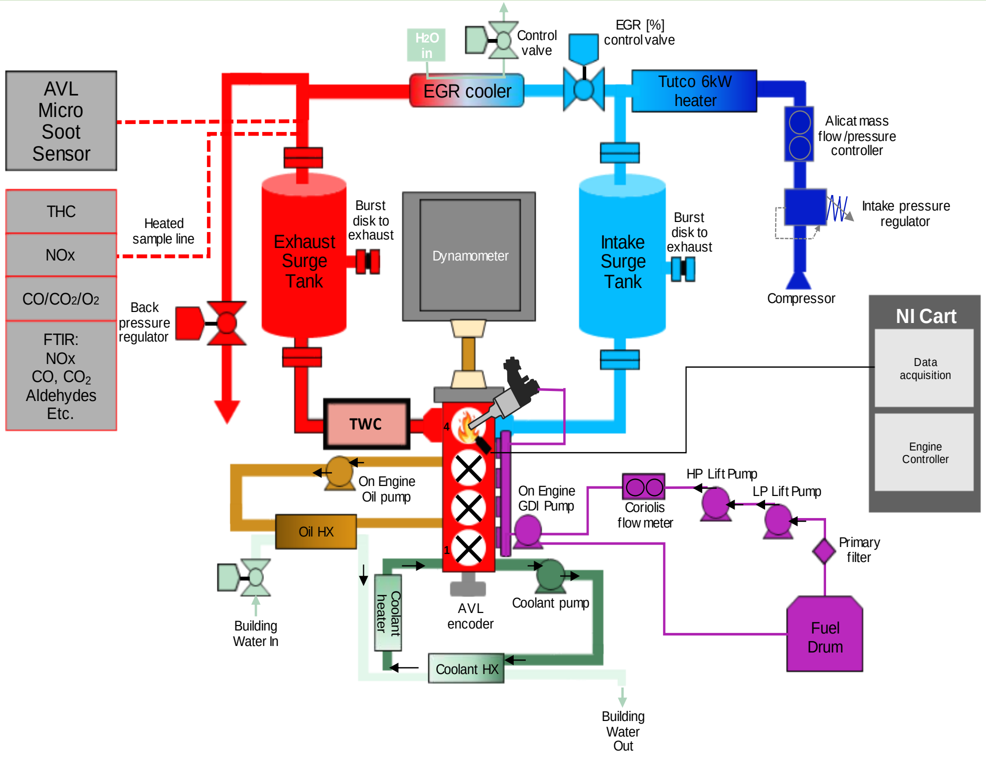
Two Tracked Milestones for FY20 that are Completed or On-Track

Task:	Effectiveness of EGR to Mitigate Knock Throughout PT Domain
Milestone:	Complete experimental knock response with 0, 10, and 20% uncatalyzed EGR at 1,500 rpm, 15 bar IMEP
Due Date:	Q2 FY20 (3/31/20)
Status:	Completed

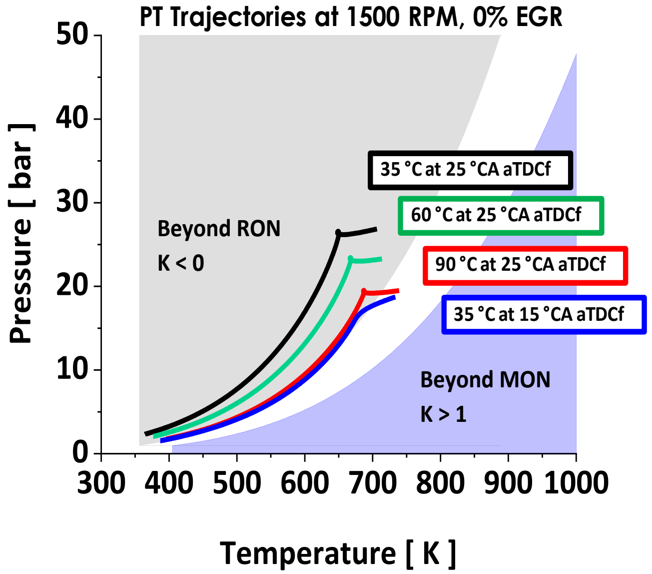
Task:	Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI
Milestone:	Validate sweep of spray-wall interaction effects on LSPI through scrape down measurements and correlate to LSPI
Due Date:	Q4 FY20 (9/30/20)
Status:	On Track

Project 1 Approach: Single Cylinder Engine to Measure Effects of EGR Effectiveness on Knock Mitigation Across Wide Range of PT Trajectory

- **GM LNF multi-cylinder engine converted to single cylinder operation**
- **Regular-grade E10 gasoline (RD5-87) and surrogate (ACE139)**
    - See technical backup slide 1 for fuel details
- **Knock-limit defined by maximum amplitude of pressure oscillation, moving to a different definition after ACEC TT feedback (see technical backup slide 2 for details)**
- **Condition selected to vary pressure-temperature trajectory, timescale (engine speed), and EGR (0-20%)**



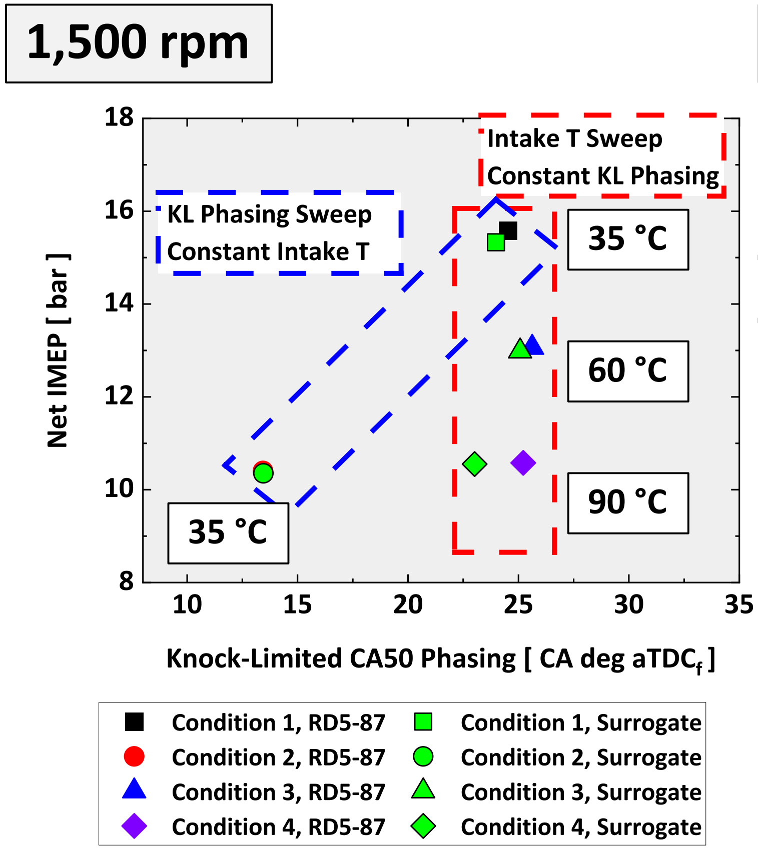
Condition	Engine Speed [rpm]	CA50 Combustion Phasing [CA aTDCf]	Intake Temperature [°C]
Condition 1	1,500	25	35
Condition 2	1,500	15	35
Condition 3	1,500	25	60
Condition 4	1,500	25	90
Condition 5	3,000	25	35
Condition 6	3,000	15	35
Condition 7	3,000	25	60
Condition 8	3,000	25	90

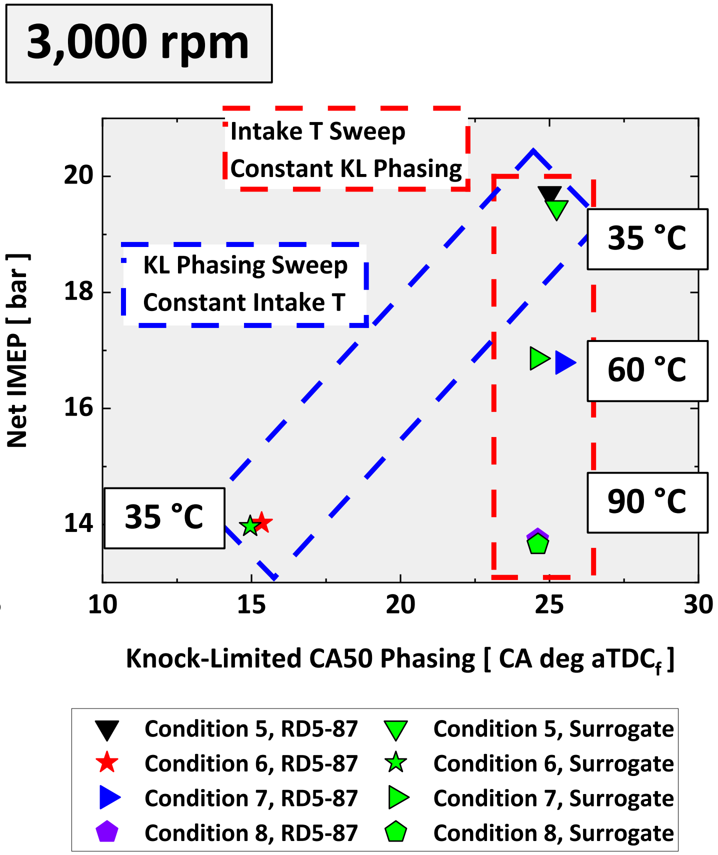


GM LNF	Value
Bore x Stroke [mm]	86 x 86
Conrod Length [mm]	145.5
Wrist pin offset [mm]	0.8
Compression Ratio [-]	Stock (9.2)
Fuel Injection System	Direct Injection, side-mounted, production injector

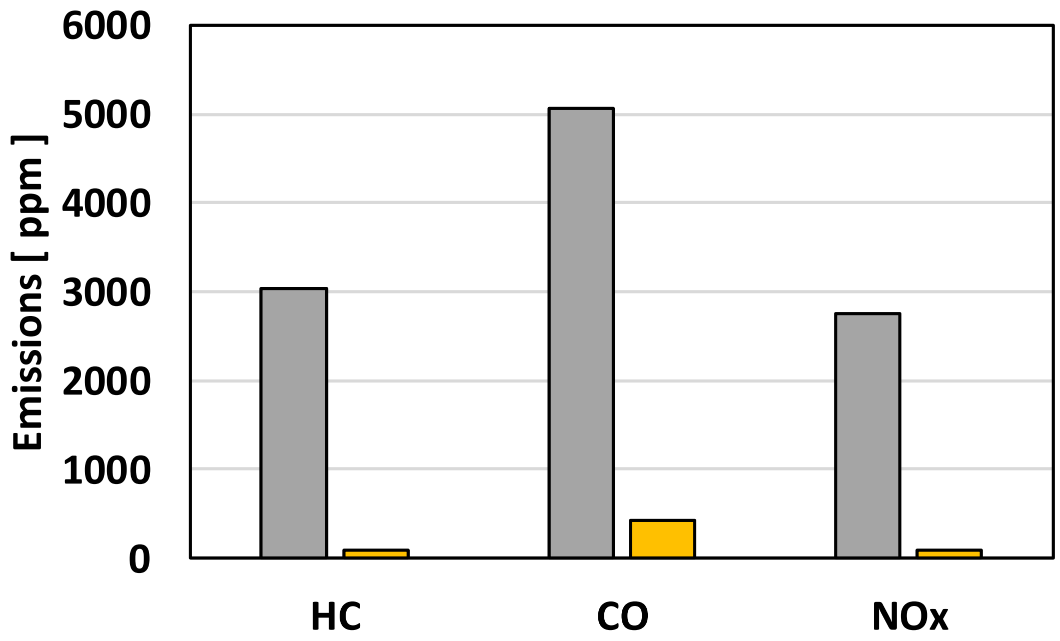
Surrogate Composition from LLNL Reproduces Baseline Gasoline over Wide Range of Engine Operating Conditions

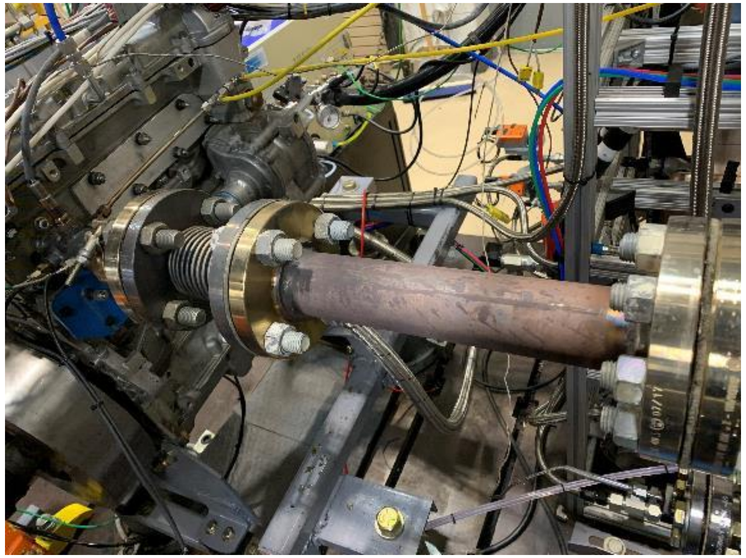
- **PACE-1 surrogate methodology and formulation described in ACE139**
- **Operating conditions varied to change kinetic boundary conditions**
  - 2x factor in engine speed
  - Intake manifold temperature varied from 35-90°C for wide range of PT trajectory
  - Differences in combustion phasing
- **Surrogate formulation reproduces knock limited combustion phasing at all conditions**
- **Surrogate formulation also reproduces cyclic variability (backup slide 3)**
- **Outcome: Surrogate formulation suitable for modeling SI knock for PACE**

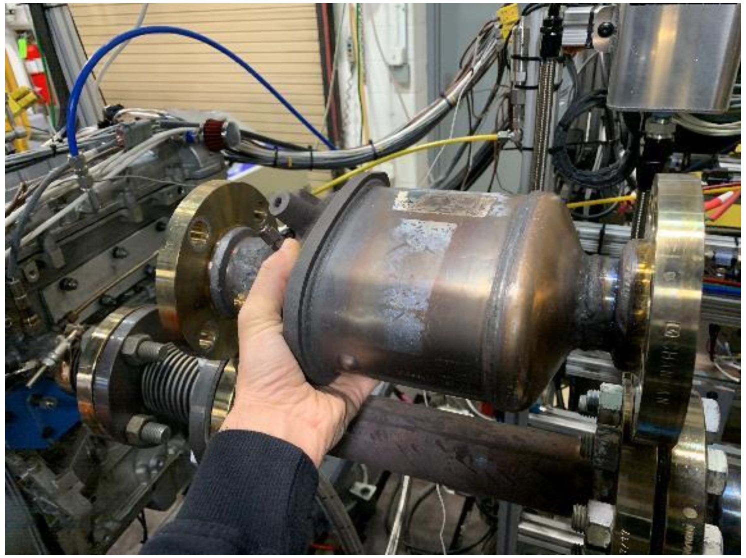




Experiments Run With and Without a Three-way Catalyst (TWC) to Alter the EGR Composition



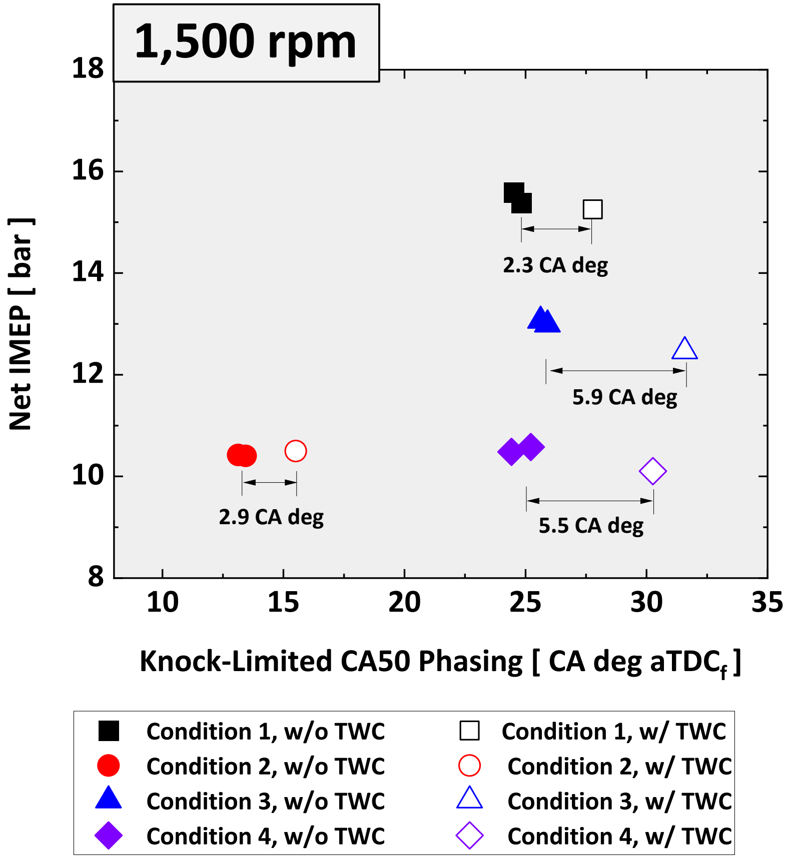


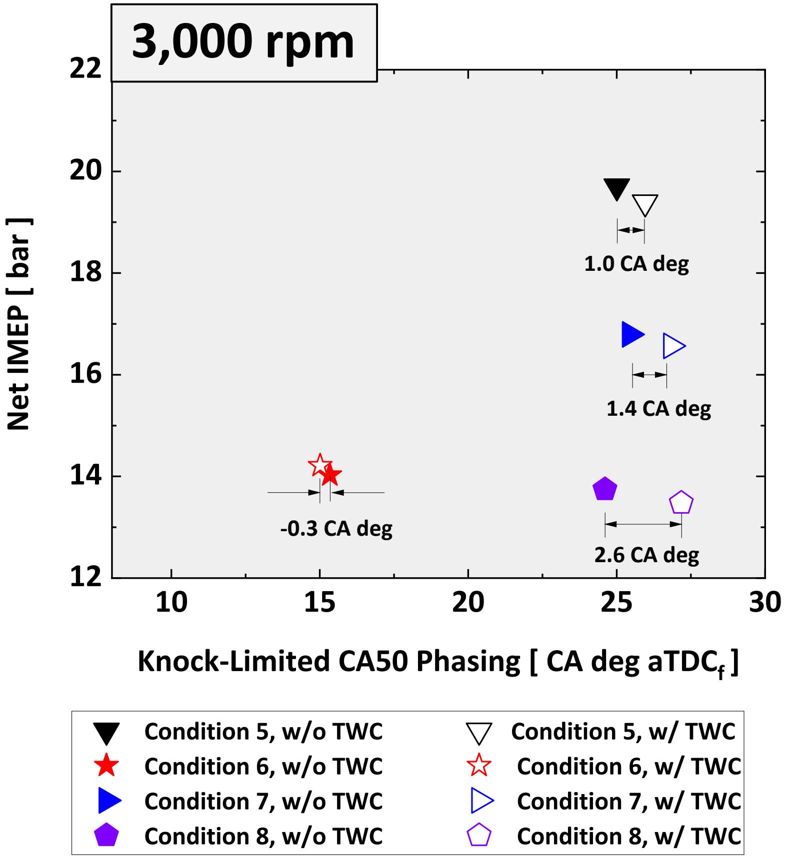


- TWC from a 2009 1.3L PZEV Chevy Malibu
- Exhaust concentrations reduced 1-2 orders of magnitude with TWC, sufficient to investigate knock-propensity impacts
- Note that lambda-dithering was not implemented for production-like emissions reduction

Presence of TWC Without EGR Caused Knock-Limit Changes due to Breathing Differences

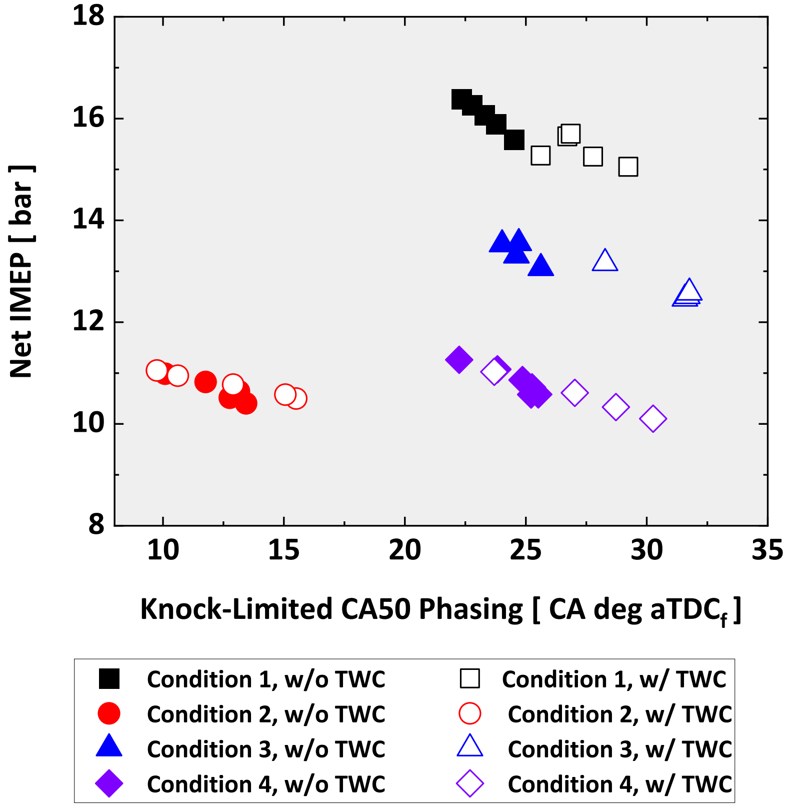
- **Knock-limit effect is more severe at 1,500 rpm where flows are lower**
  - Not strictly a backpressure/ increased flow effect
  - Possibly due to wave dynamics
  - Possibly due to kinetic sensitivities (more time for knock to occur at 1,500 rpm)
- **Regardless of cause, different knock-limited phasing at 0% EGR must be accounted for**

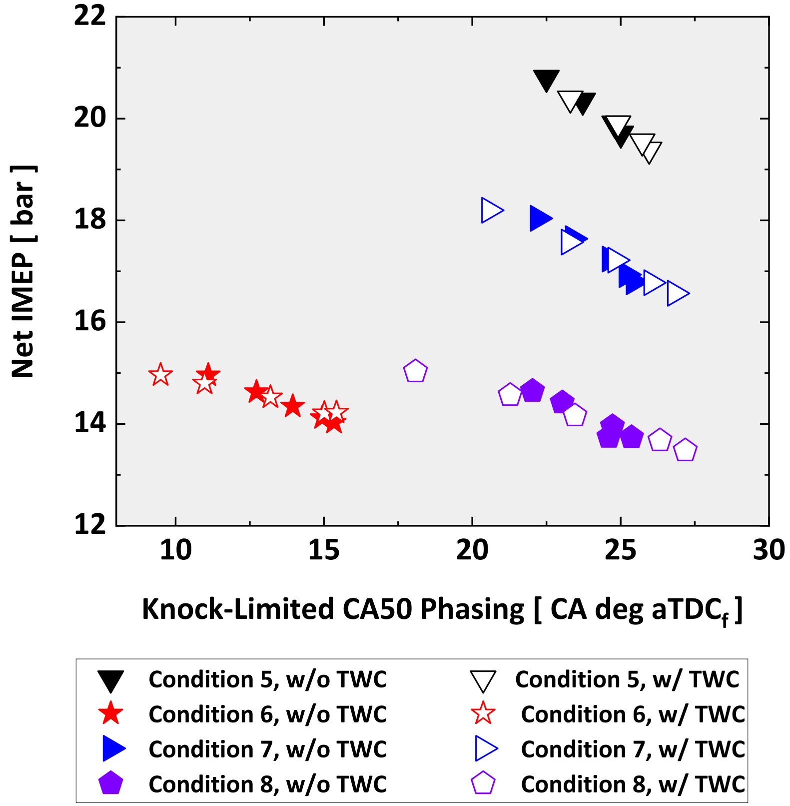




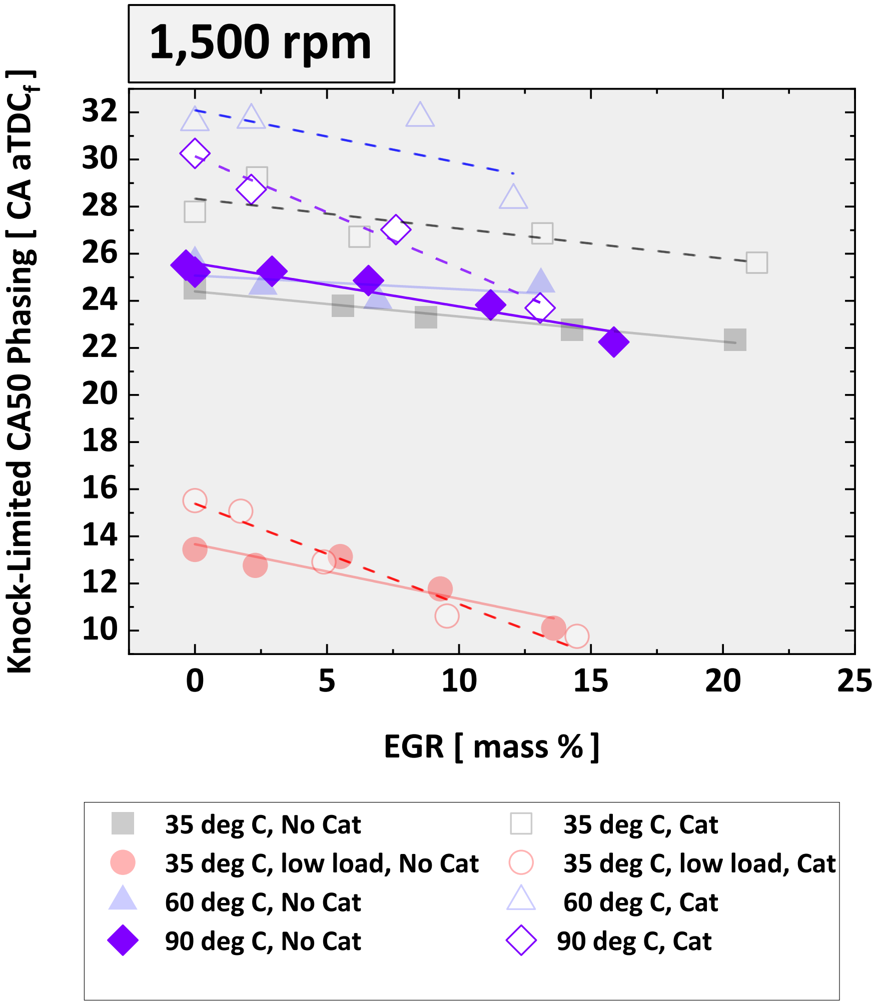
Addition of EGR Allows Combustion Phasing Advance at All Conditions; Extent of Advance is Condition Dependent

- **Knock-limited combustion phasing advances at all conditions**
  - Net effect of numerous competing effects of EGR (see technical backup slide 4)
- **Engine load also increases at all conditions**
  - Constant air and fuel flow
  - Load increase due to higher efficiency
  - Higher efficiency due to more advanced phasing, higher γ, reduced heat losses
- **Effectiveness of EGR for knock mitigation each condition can evaluated**





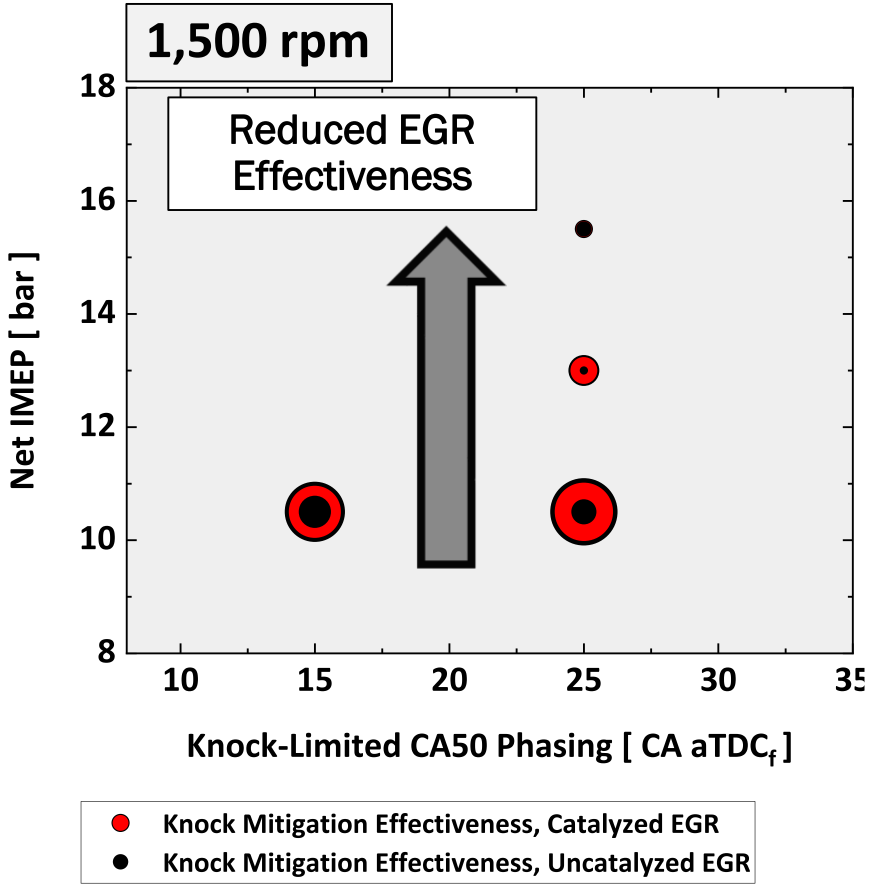
Effectiveness of EGR to Mitigate Knock can be Analyzed by Linear Regression

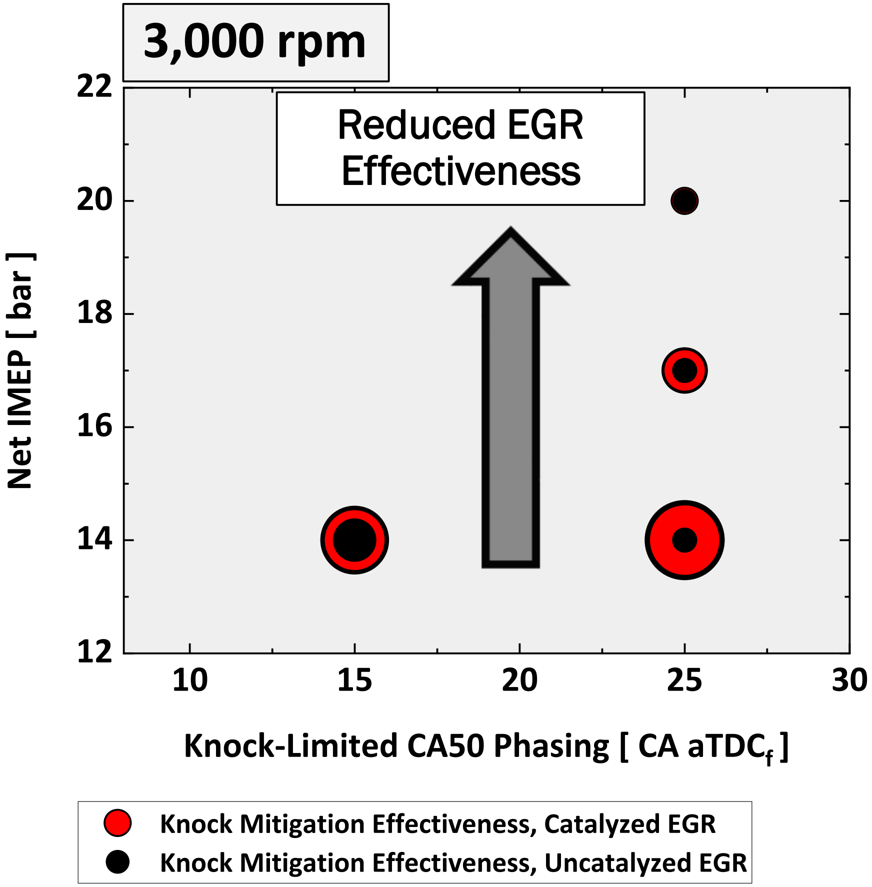


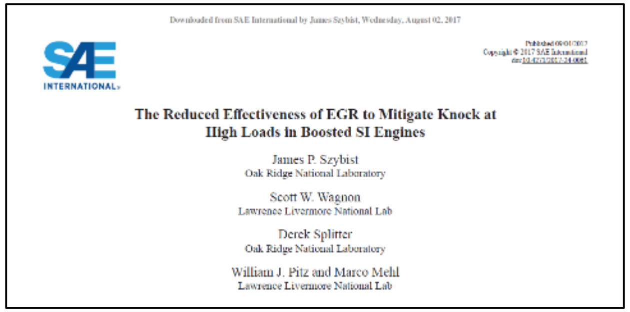
	Cat/ No Cat	KL CA50 Advance/% EGR
1500, 35, low	No Cat	0.23
	Cat	0.43
1500, 35, high	No Cat	0.11
	Cat	0.13
1500, 60, low	No Cat	0.06
	Cat	0.22
1500, 90, low	No Cat	0.18
	Cat	0.48

Visualization of EGR Knock Effectiveness with Bubble Chart Illustrates Effect of Load and Catalyzed EGR

- **Bubble diameter is proportional to knock mitigation effectiveness (CA deg / % EGR)**
- **EGR effectiveness decreases for boosted conditions**
- **This is consistent with previous findings regarding PT trajectories across a wider range of conditions**







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The Reduced Effectiveness of EGR to Mitigate Knock at High Loads in Boosted SI Engines

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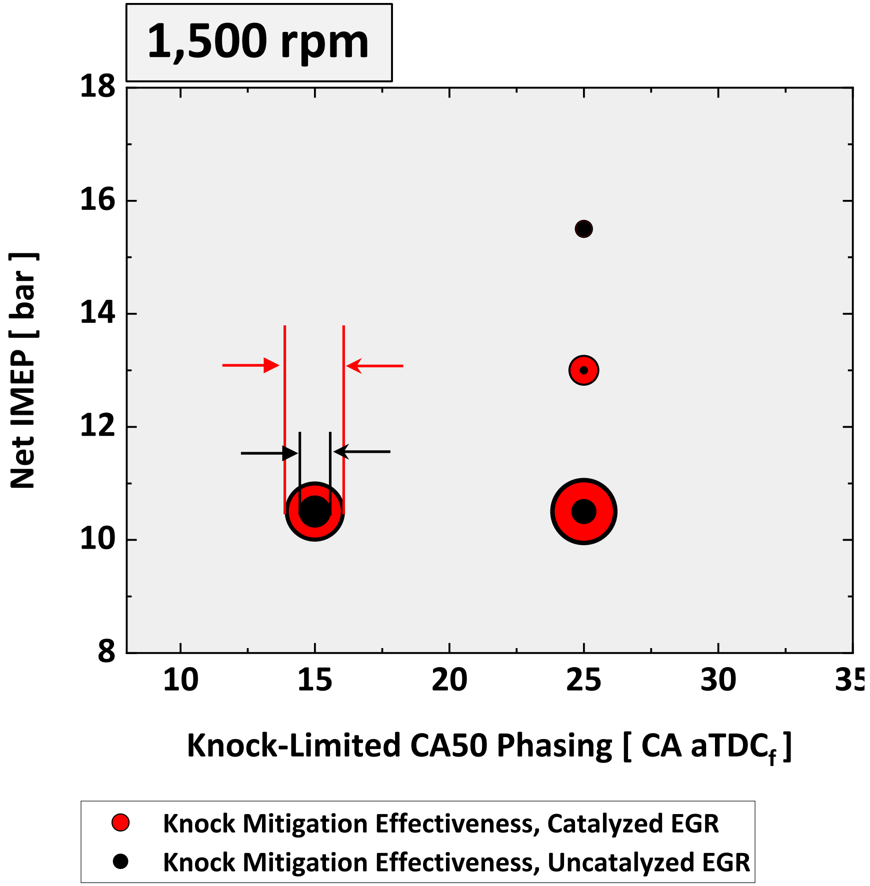
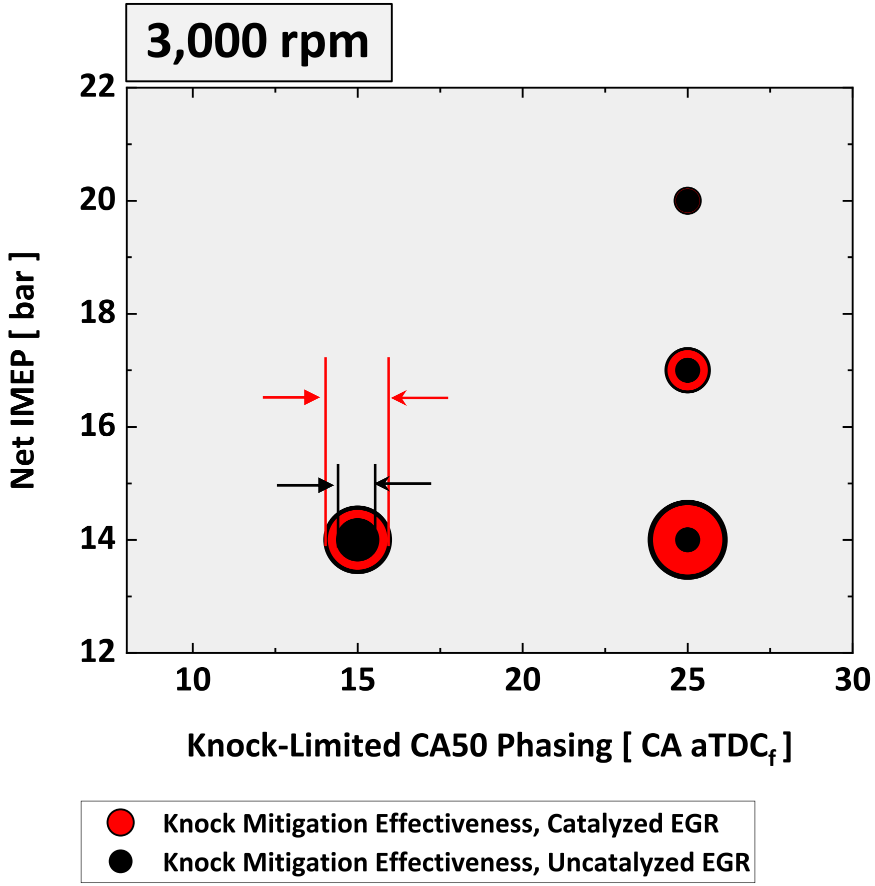
Catalyzed EGR Performs Significantly Better than Non-Catalyzed

- Catalyzed EGR removes NOx and HC, which can increase reactivity
- Catalyzed EGR appears to be most effective for high intake / later phasing condition
- Based on analysis of concentrations, reactivity difference is likely due to NO rather than minor HC constituents
- Complete details are reported in draft manuscript submitted to SAE 2020 Fall PFL meeting





Motivation Project 2: Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI

- Recent Co-Optima found that dilution of oil with fuel changed the LSPI tendency
  - Dilution of oil inferred from decrease of oil pressure through LSPI test
- One hypothesis that fuel/oil composition and chemistry in crevice is important for LSPI
  - Nitrogenation can occur in this region under some conditions
  - Nitrogenated compounds are sensitive to alkali and alkaline metal additives in lube
- Oil pressure is an attenuated measurement of oil dilution
  - Represents oil sump condition, not top ring and crevice condition
  - More direct measurement of cylinder scrape-down is desired

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Fuel-Lubricant Interactions on the Propensity for Stochastic Pre-Ignition

Derek Splitter, Brian Kaul, and James Szybist Oak Ridge National Laboratory

Lake Speed Driven Racing Oil

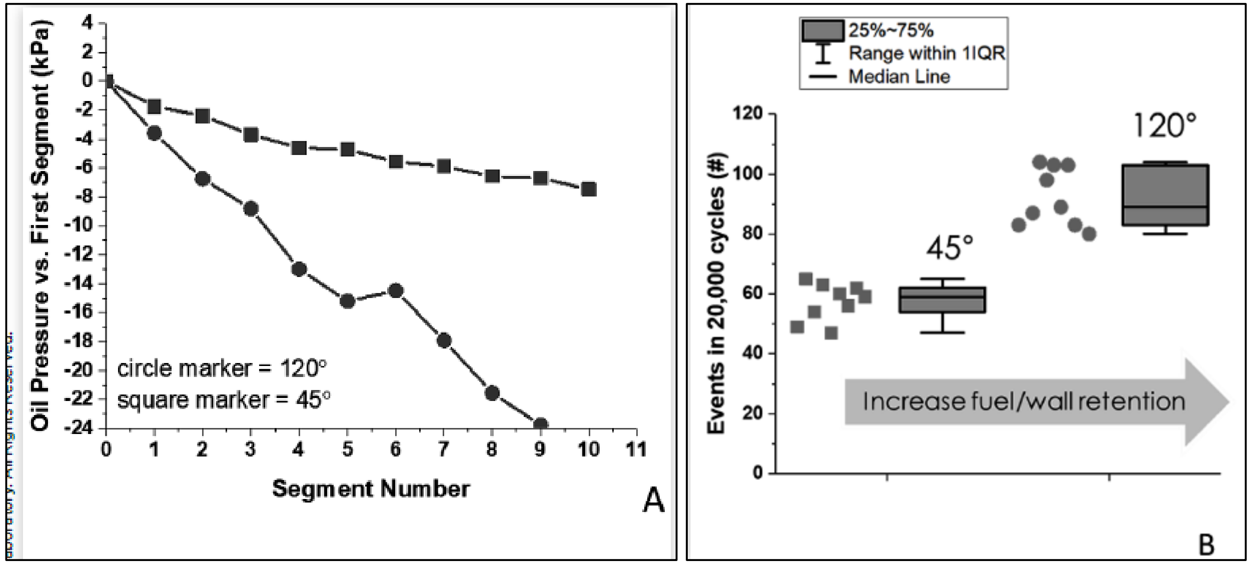
Bradley Zigler and Jon Luecke National Renewable Energy Laboratory

Citation: Splitter, D., Kaul, B., Szybist, J., Speed, L. et al., "Fuel-Lubricant Interactions on the Propensity for Stochastic Pre-Ignition," SAE Technical Paper 2019-24-0103, 2019, doi:10.4271/2019-24-0103.

Abstract

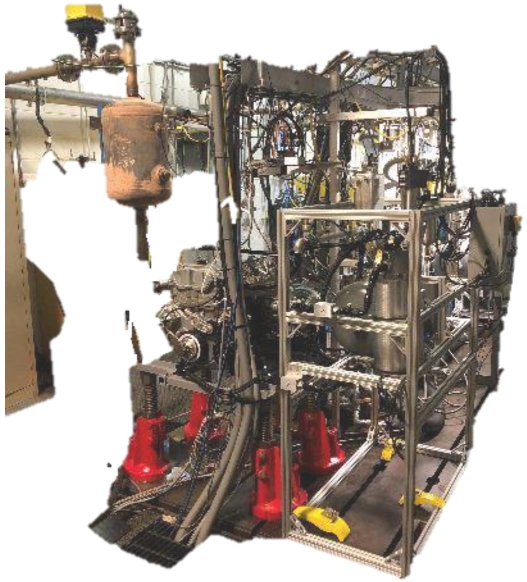
This work explores the impact of the interaction of lubricant and fuel properties on the propensity for stochastic pre-ignition (SPI). Findings are based on statistically significant changes in SPI tendency and magnitude, as deter-

detergent effects could be observed even at reduced loads. This suggests that there is a thermal effect associated with the higher load operation. It was hypothesized that the thermal effect was associated with lube oil nitrogenation. To test this theory, nitromethane (CH_3NO_2) was blended at 6.5% by

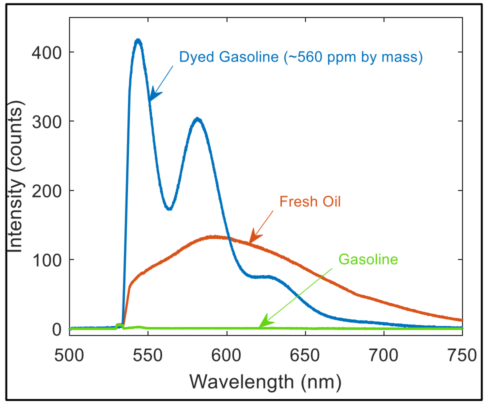


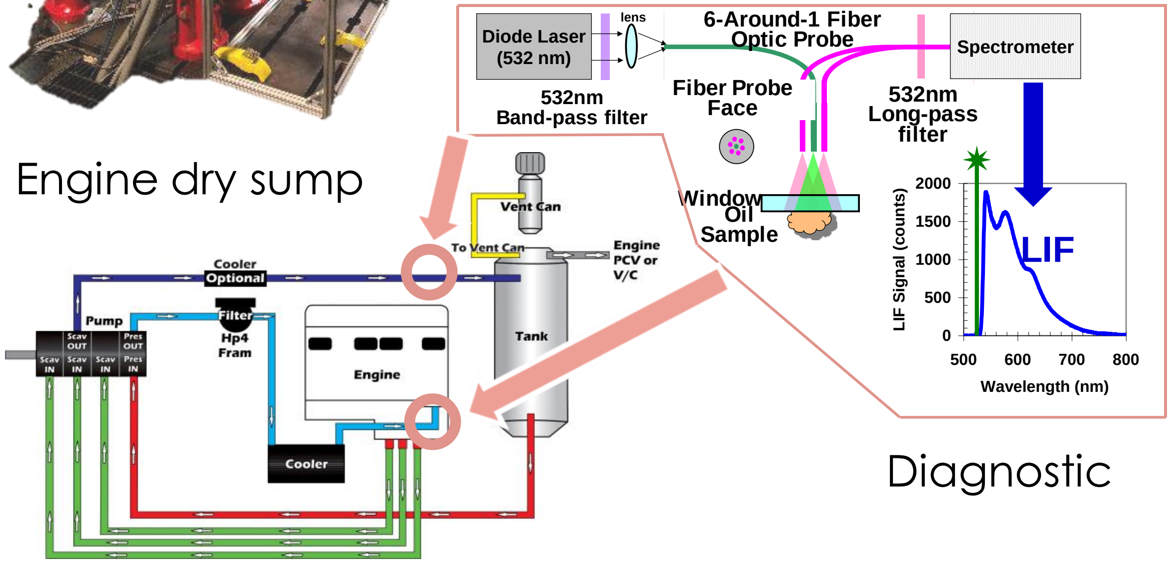
Experimental LSPI Approach Focuses on Fuel-Wall Interaction and Liquid Retention as Potential Source of LSPI

- Quantification of fuel effects on fuel-wall interaction at high load
  - Apply LIF diagnostic to quantify fuel-oil dilution in the oil returning from top ring zone
- GM LNF 2.0L engine converted to single cylinder with dry sump oiling system
  - Same geometry show on slide 5
  - ORNL control system for LSPI testing using automated test sequence (10 segments, 25,000 cycles per segment)
  - Dry sump reduces sump dilution of oil for LIF, increased signal, reduced run time for signal
- Dye-based LIF diagnostic developed at ORNL
  - Previously developed as part of ACE032
  - Diagnostic received 2013 R&D 100 Award
- Experiments will also verify that PACE-1 gasoline surrogate fuel has similar retention (ACE139)



Engine dry sump



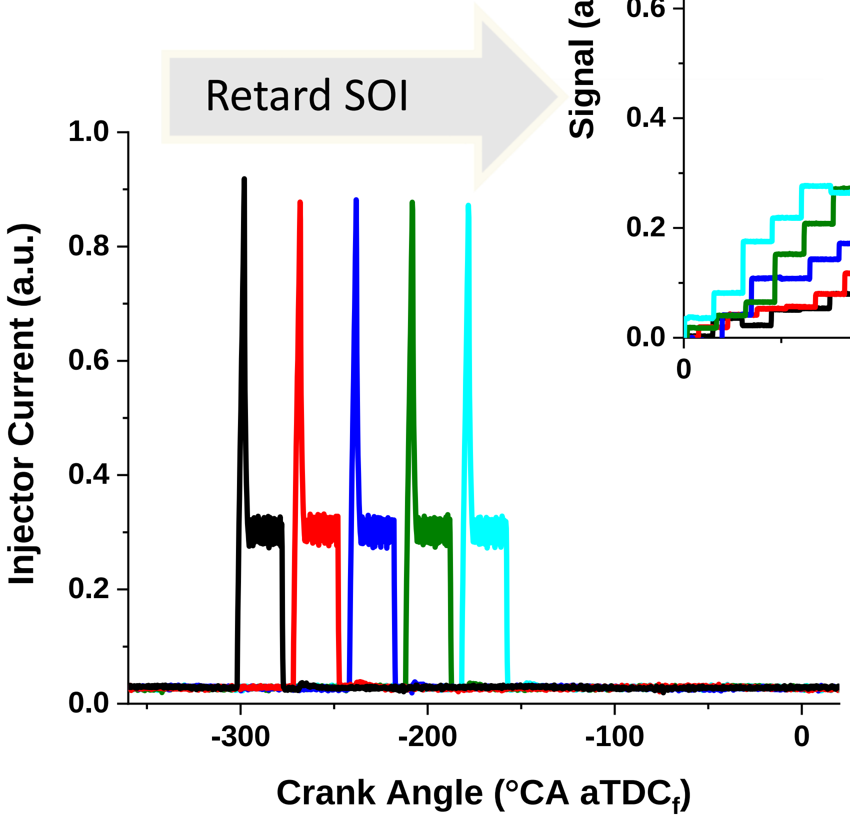


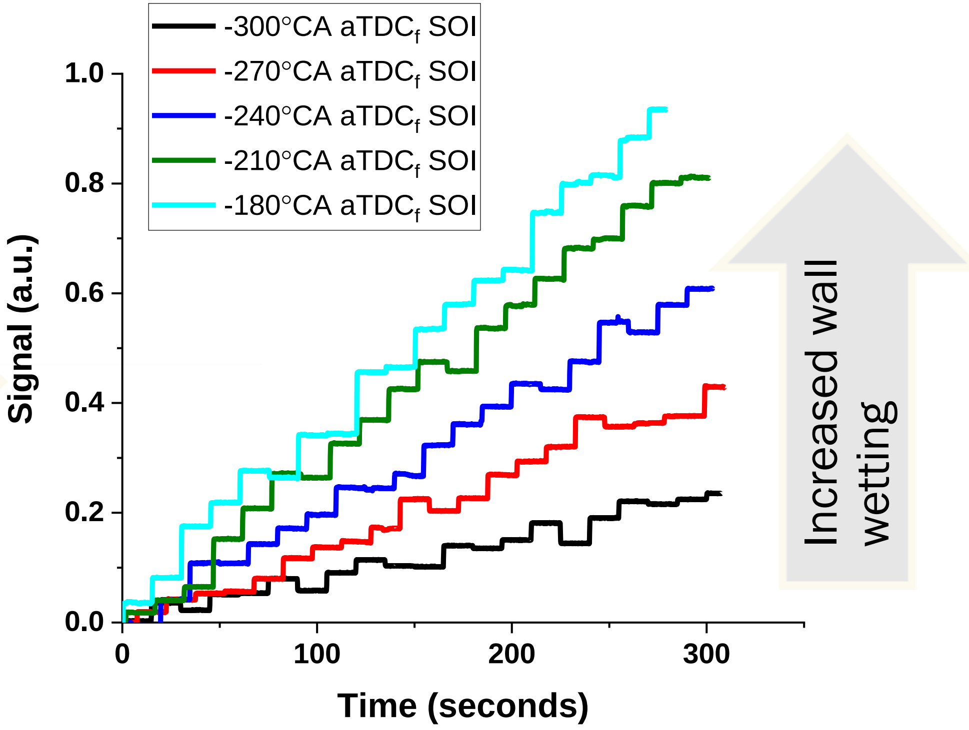
Diagnostic

Application of LIF Diagnostic is On-Track. Preliminary Results Show Fast Response and Directionally Correct Trends

- Initial application for fuel injection timing sweep at 10 bar IMEP
- 500 ppm dye in fuel
  - Dye level found to be excessive
- Fuel accumulation in oil increases with retarded SOI timing
  - Thought to be due to reduced evaporation time
  - PACE spray project (ACE 143 and ACE 144) to refine conceptual understanding

Initial results show diagnostic capturing fuel retention trends





Injection timing sweep shows quick signal response on the order of seconds

Responses to Previous Year Reviewers' Comments

- **This work has not been previously reviewed.**

Collaboration and Coordination with Other Institutions

- PACE is a collaborative project of multiple National Laboratories that combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions.
- The work plan for PACE is developed in coordination with the USDRIVE Advanced Combustion and Emission Control (ACEC) Tech Team
- Individual collaborations for this project:
  - Surrogate collaboration: LLNL, SNL, ANL
  - Machine learning for LSPI: Data set supplied by Lubrizol. Machine learning ongoing.
  - Related funds-in LSPI project with CRC

Remaining Challenges and Barriers

- **PACE-wide barriers discussed in ACE138**
- **Causes of increased EGR effectiveness after treatment with TWC are unclear**
  - Not clear what individual compound or combination of compounds cause this effect
  - Uncertain whether this sensitivity is accurately captured by kinetic models
  - Can this effect accurately be predicted by CFD models? This project will provide data for validation and verification for CFD model development.
- **Not clear how much fuel impingement is needed to cause LSPI propensity to increase**
  - How much can we improve fuel injection strategies to reduce LSPI?
- **What are the liquid-phase dependencies and what chemistry occur in the crevice region to cause LSPI?**
  - What role do lube oil additives play?
  - What are the required thermodynamic conditions?
- **Can machine learning be used to predict next-cycle knocking and/or LSPI events?**

Proposed Future Research Includes Broader PACE Interactions

Any proposed future work is subject to change based on funding level

Project 1. Effectiveness of EGR to Mitigate Knock Throughout PT Domain (ORNL, Szybist)

FY20 Results Presented on Slides 5-12

FY 20 Results Inform FY21 Experiments Seeding Individual Components Into TWC-Treated EGR (NO, C_2H_2, C_2H_4)

Kinetic Modeling of Results, relying on Support and Collaboration with LLNL Kinetic Modeling Effort (Wagnon, ACE139)

Machine Learning and Deterministic Patterns (Kaul, ACE148)

CFD Modeling of Knocking Combustion (Edwards, ACE150)

Project 2. Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI (ORNL, Splitter)

Complete FY20 Investigation (on-track)

Continuing FY21 Investigations to Characterize Oil Dilution

Spray Strategies for Reduced Fuel-Wall Impingement (Pickett, ACE144)

Machine Learning and Deterministic Patterns (Kaul, ACE148)

Surrogate Development Feedback on Oil Dilution (Wagnon, ACE139)

Summary Slide

Relevance

- Overall goals of PACE are to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions
- Mitigation of knock and LSPI are the top barrier to attaining higher efficiency for dilute SI combustion in USDRIVE roadmap

Approach

- SCE experiments to measure effectiveness of EGR on knock mitigation over a large dimension space (PT trajectory, timescale, w/ and w/o TWC)
- LSPI investigations to measure fuel dilution of lubricating oil
- Outputs of these experimental investigations feeding into other PACE efforts: machine learning, CFD modeling, kinetic model development, more

Accomplishments

- Confirmed that EGR is less effective at mitigating knock under boosted conditions than naturally-aspirated conditions, regardless of engine speed
- Illustrated that EGR treated with a TWC is more effective at mitigating knock than untreated EGR
- Completed setup of an LSPI experiment to directly measure fuel dilution of oil scrape-down using an optical diagnostic technique

Collaborations

- PACE is a collaboration of 6 National Laboratories, workplan developed considering input from ACEC TT, code developers, and more
- PACE projects presented at AEC semi-annual program review meeting
- Numerous project-level collaborations direct with industry and industry consortia for support and feedback

Future Work

- Investigations to determine the role of individual minor constituents of EGR play on knock propensity, collaborating with LLNL kinetics team
- Continue LSPI investigations of fuel oil dilution, including impact of spray strategy and matching of surrogate composition
- Make data from these projects available to advance PACE more broadly: machine learning, CFD modeling, kinetics development, and surrogate development

Technical Back-up Divider Slide

Technical Backup Slide 1. Fuels and Fuel Properties

- **Regular-grade E10 research gasoline was used for this study (product name RD5-87 from Gage Products)**
- **Gasoline surrogate (PACE-1) also blended and tested at 0% EGR conditions**
  - PACE-1 surrogate development presented in ACE139
- **Actual concentrations for PACE-1 fuel blended at ORNL are shown in Table 1**
- **Measured fuel properties for Gasoline and PACE-1 shown in Table 2**

Table 1. Desired and actual blended concentrations for PACE-1 surrogate fuel.

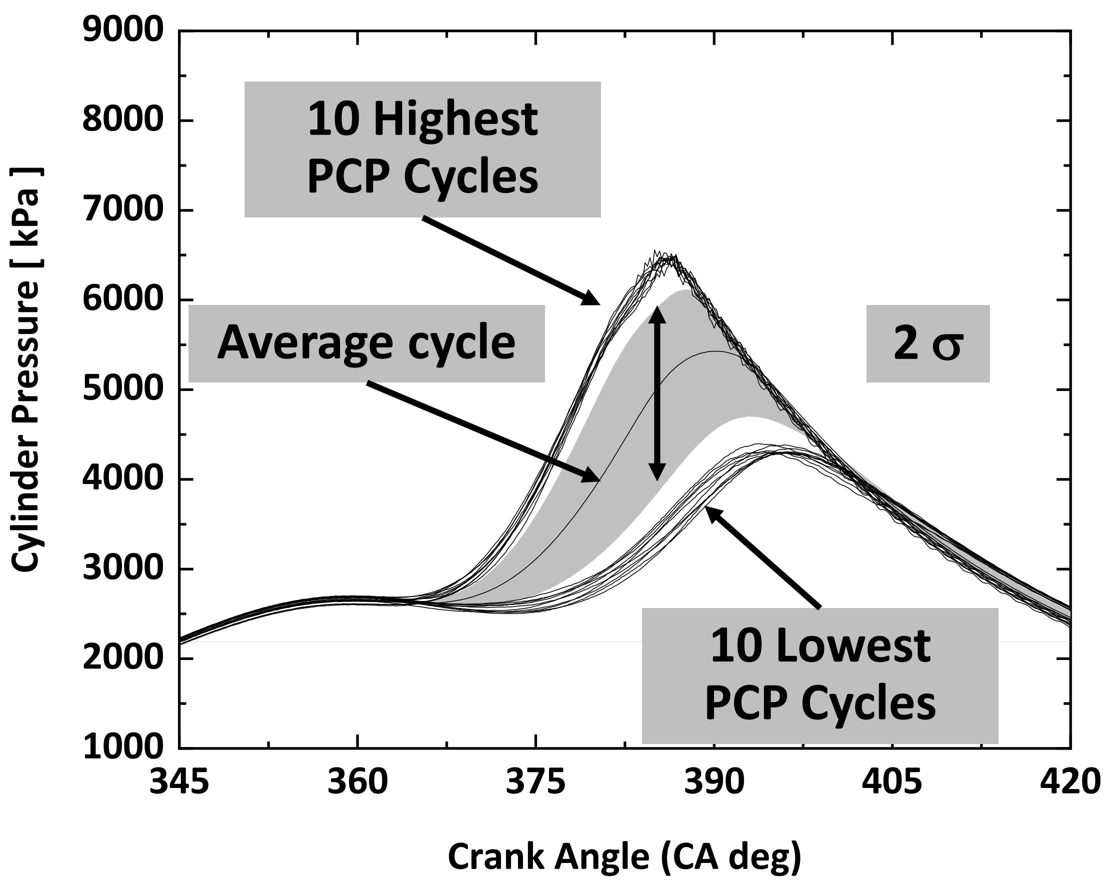
	Desired Mass %	Actual Mass %	Error %
n-heptane	17.13	17.12	-0.06
iso-pentane	6.35	6.37	0.37
iso-octane	19.89	19.90	0.05
1-hexene	5.97	5.97	-0.06
Cyclopentane	10.60	10.60	-0.03
1,2,4-trimethylbenzene	30.11	30.09	-0.06
Ethanol	9.95	9.95	0.03

Table 2. Measured fuel properties for gasoline (RD5-87) and PACE-1 surrogate.

	Method	Gasoline RD5-87	Surrogate PACE-1
Research Octane Number [-]	ASTM D2699	92.3	92.3
Motor Octane Number [-]	ASTM D2700	84.6	82.4
Octane Sensitivity [-]	RON – MON	7.7	9.9
Initial boiling point [°C]	ASTM D86	40.4	44.4
T10 [°C]	ASTM D86	54.8	59.4
T50 [°C]	ASTM D86	101.3	98.9
T90 [°C]	ASTM D86	157.9	165.0
Final boiling point [°C]	ASTM D86	172.1	165.6
Specific Gravity [-]	ASTM D4052	0.75	0.75
Carbon [wt %]	ASTM D5291	82.67	82.52
Hydrogen [wt %]	ASTM D5291	13.66	13.65
Oxygen [wt %]	ASTM D5599	3.51	3.38
Stoichiometric Air-Fuel Ratio	Calculated	14.2	14.5
Lower Heating Value [MJ/kg]	ASTM D4809	41.93	41.81
Aromatics [wt %]	ASTM D6729	27.9	30.3
n-Saturates [wt %]	ASTM D6729	13.9	17.2
Iso-Saturates [wt %]	ASTM D6729	29.0	26.2
Olefins [wt %]	ASTM D6729	5.5	5.8
Naphthenes [wt %]	ASTM D6729	12.4	10.2
Ethanol [wt %]	ASTM D5599	10.12	9.74

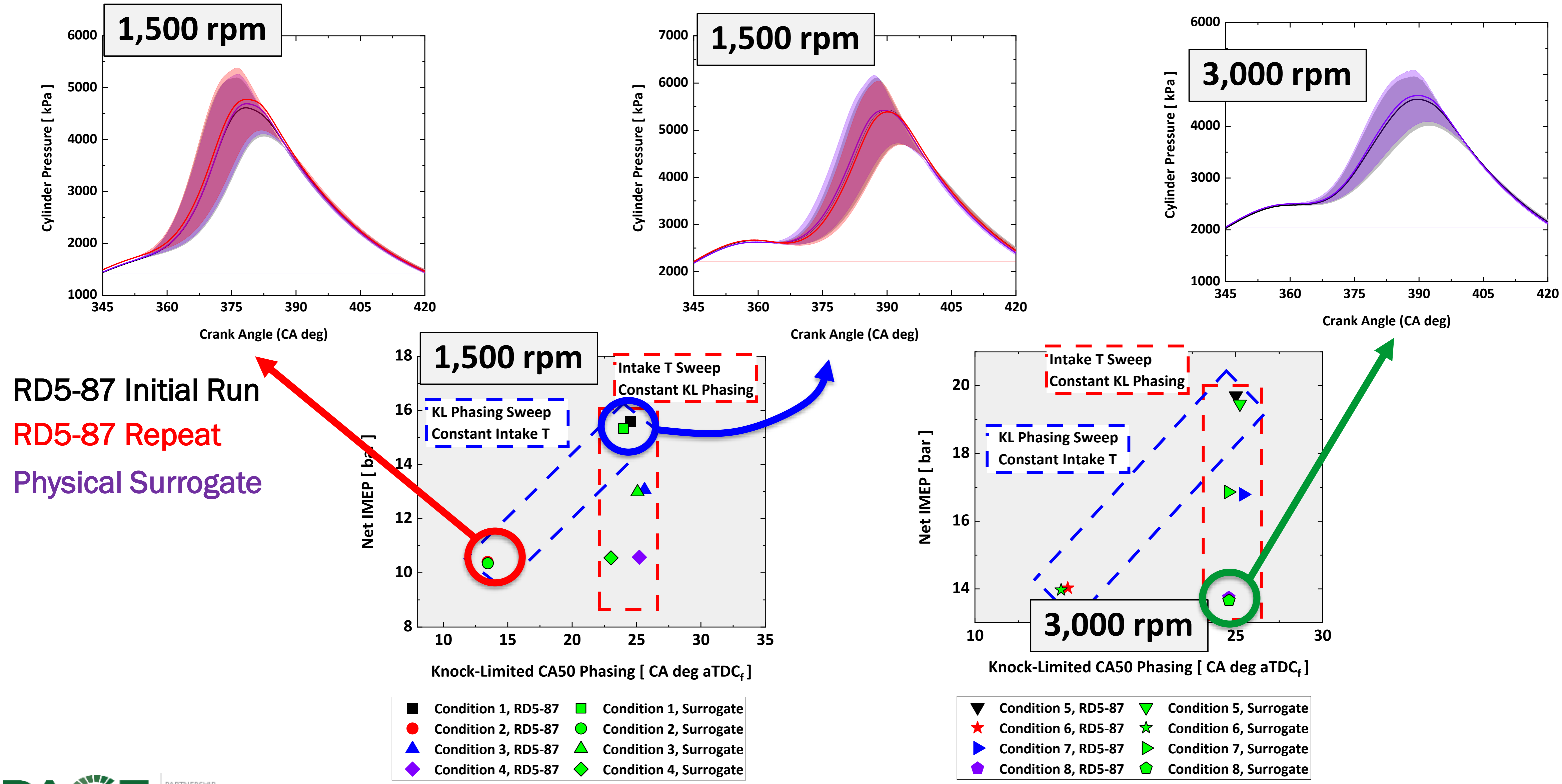
Technical Backup Slide 2. Knock Defined by Threshold MAPO for the Highest 10% Peak Cylinder Pressure (PCP) Cycles

- **Only a fraction of engine cycles knock under a knocking condition**
- **Including all cycles in maximum amplitude of pressure oscillation (MAPO) threshold can be misleading, particularly with EGR**
  - Higher cycle-to-cycle variability with EGR
  - Average of all cycles allows permits heavy-knocking cycles
- **MAPO threshold applied:**
  - 1,500 rpm: 30 kPa for highest 10% of PCP cycles
  - 3,000 rpm: 60 kPa for highest 10% of PCP cycles



NOTE: Since the conclusion of this investigation, we have been working with the ACEC TT to develop a revised definition of knock for PACE that will work for both experiments and simulations. This will rely on the power spectrum density, have a threshold that increases with engine speed, and have a weighting factor.

Technical Backup Slide 3. RD5-87 and PACE-1 Surrogate have Matching Cyclic Variability, as shown by the 2σ Variability at Three Different Conditions



PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Technical Backup Slide 4: Competing Thermodynamic Effects of EGR

Good for Knock Mitigation

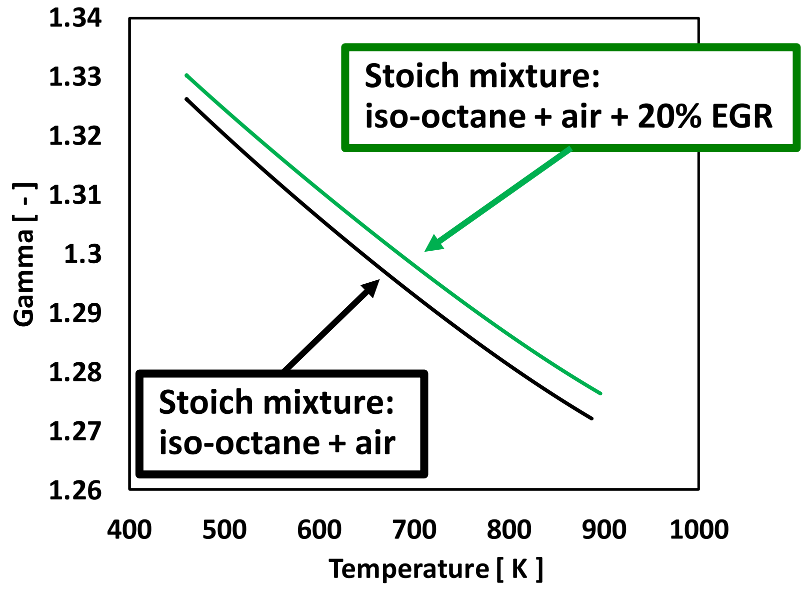
- Reduce the burned gas temperature
- Slower kinetics?

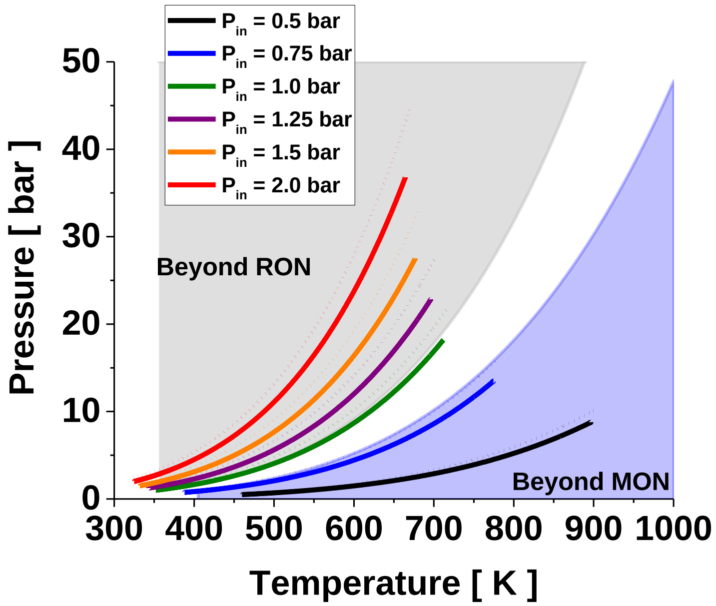
Bad for Knock Mitigation

- Increased P due to higher mass at IVC
- Increase gamma during compression (higher unburned gas T)
- Increase burn duration (longer time for mixture to "cook")

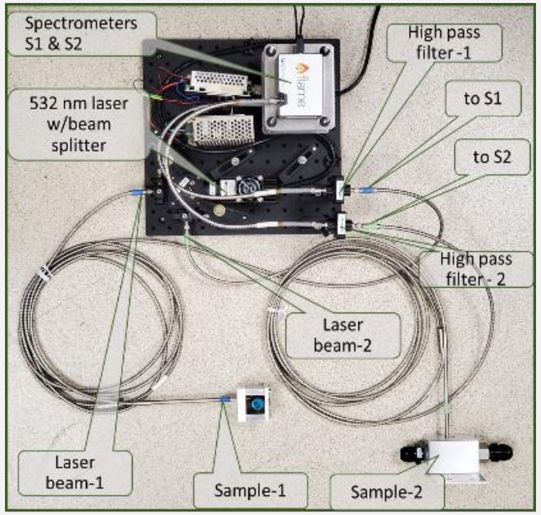
Prior work details the extent of pressure and temperature increase in unburned gas with 20% EGR

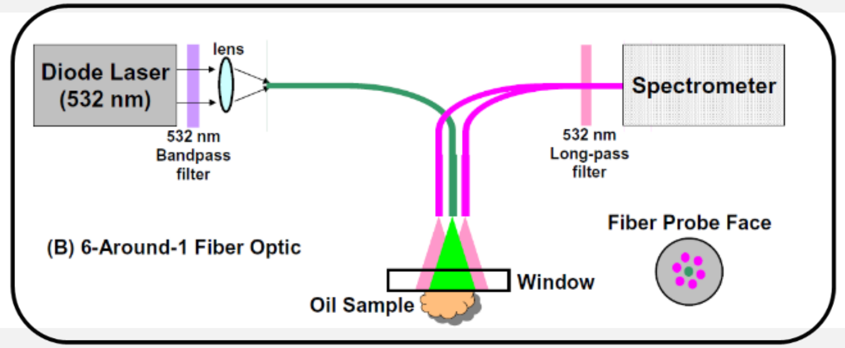
- SAE 2017-24-0061
- Compressive temperature increase up to 35 K
- Compressive pressure increase up to 7 bar





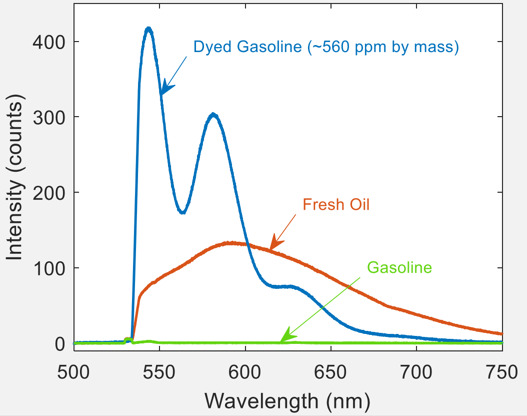
Technical Backup Slide 5. Quantitative Dye-Based LIF Diagnostic Developed to Measure Fuel in Oil in Prior Years as part of ACE032



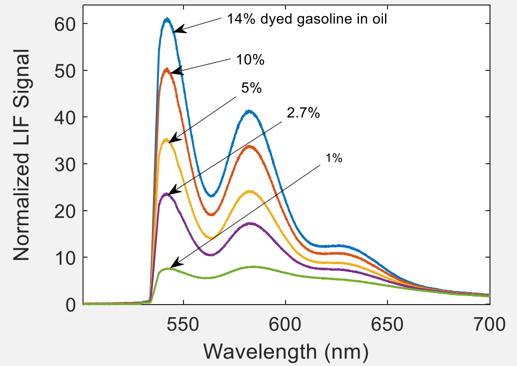


LIF experiment setup utilizing a **532-nm laser diode** as an excitation source; **6-around-1 fiber-optic probes**; and Ocean Optics Flame-T spectrometers (via **high-pass filters** to block residual laser light)

Spectra of Gasoline, Oil and Dye



Spectra at different dyed gasoline concentration



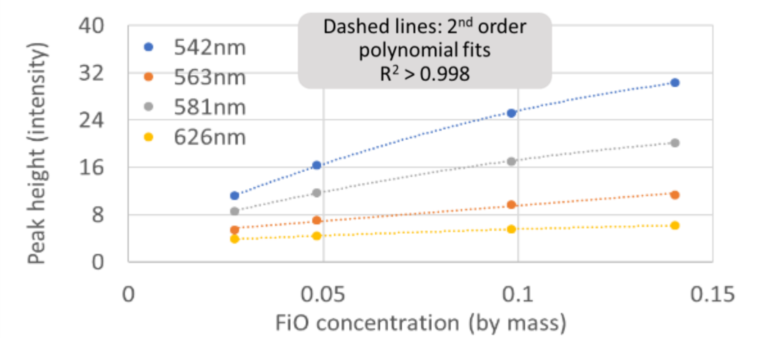
Model-Based Calibration

$$A_\lambda = k_{\lambda,0} + k_{\lambda,1}.x + k_{\lambda,2}.x^2$$

$$\begin{bmatrix} A_{11} & \dots & A_{1p} \\ \vdots & \dots & \vdots \\ A_{n1} & \dots & A_{np} \end{bmatrix} = \begin{bmatrix} k_{11} & k_{12} & k_{13} \\ \vdots & \vdots & \vdots \\ k_{n1} & k_{n2} & k_{n3} \end{bmatrix} \times \begin{bmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_p \\ x_1^2 & \dots & x_p^2 \end{bmatrix}$$

Solve for calibration coefficients

$[k] = [A]^* [x]^+$



Bench Validation and Verification